# MODELING OF BIOCHEMICAL NETWORKS IN CELLS WITH MONTE CARLO SIMULATION

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PROJECT

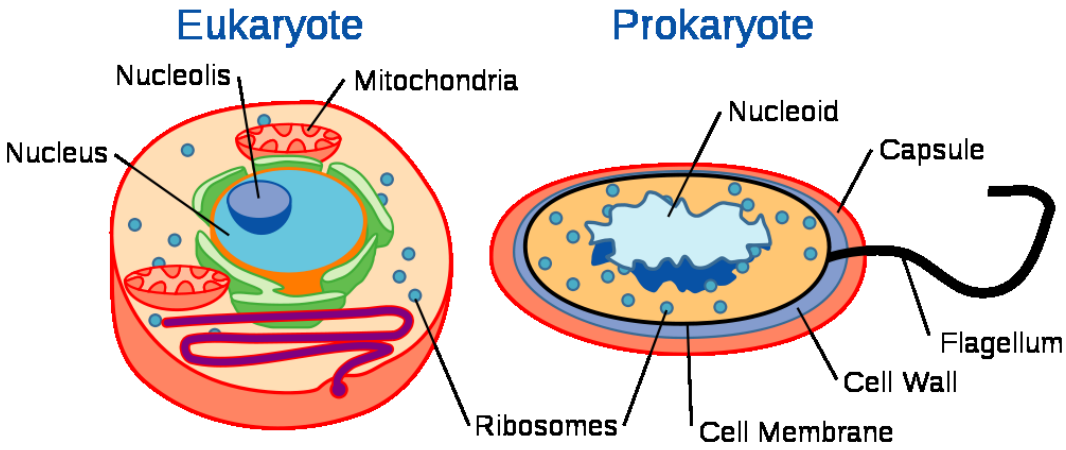


FIGURE 1. A eukaryote cell (e.g. a mammal cell) and a prokaryote cell (e.g. a bacterium) Source: Wikipedia

The interest in computer simulations of processes in living cells is increasing in an effort to understand the very complicated biochemical network in a cell. The molecules in a cell move in space by diffusion and react with each other to form new compounds.

According to classical macroscopic chemistry, the concentrations of reacting substances generally obey deterministic rate-diffusion laws in the form of differential equations. In living cells, however, the number of molecules of the chemically active molecules such as proteins is often low and reactions between the molecules are more accurately described by a *random* process [1]. The molecules are diffusing more or less freely inside the cell by random Brownian motion and reactions are scheduled as random events. For some processes it is possible to assume that the system is *well stirred* and we can ignore the space dependence of the solution.

There is a differential equation called the *master equation* for the probability density function of the molecules. The solution $p(\mathbf{x}, t)$ to the equation is time dependent and is the probability that there are $\mathbf{x}$ molecules at time $t$. Since the dimension of $\mathbf{x}$ often is high the master equations suffers from the *curse of dimensionality* and cannot be solved numerically. It is possible to simulate the system with a Monte Carlo method [3] and

approximate the mean values, the variations, and the correlations of the process as in [4]. Good approximations can be obtained on a coarser mesh in the molecular space and by combining the solutions on the different meshes.

The purpose of this project is to test the Monte Carlo method on coarser meshes and compare with the solution of the master equation in particular to compute the steady state distribution. The test cases will be such that the dimension of the system is not a problem.

## References

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[3] D. T. Gillespie, A general method for numerically simulating the stochastic time evolution of coupled chemical reactions, *J. Comput. Phys.*, 22 (1976), 403–434.

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